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Chapter 21

BIOSCREEN, AT123D, AND MODFLOW/MT3D, A COMPREHENSIVE REVIEW OF MODEL RESULTS

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ABSTRACT

The Domenico equation is commonly used to evaluate long term risks associated with contaminated groundwater. Numerous groundwater models are based on it, including BIOSCREEN and BIOCHLOR. This paper compares the results from BIOSCREEN, AT123D and MODFLOW/MT3D groundwater models. Results from the AT123D and MODFLOW/MT3D models indicate that BIOSCREEN significantly underestimates contaminant mobility and thus exposure risks. This was unexpected as BIOSCREEN results are commonly assumed to be extremely conservative. In fact BIOSCREEN did produce the highest downgradient concentrations; however it took unreasonably long periods of time to achieve them. Such lengthy time periods are not typically evaluated as part of a risk evaluation. Even more surprisingly, BIOSCREEN produced the same peak concentration for all contaminants and for all aquifer types tested. Both contaminant concentration and travel times from AT123D and MODFLOW/MT3D models were almost identical. Furthermore, these results varied with contaminants and aquifer properties as expected. The influence of biodegradation was also evaluated. Inclusion of conservative biodegradation rates made BIOSCREEN the least conservative model by far. This is because the lengthy travel times produced by BIOSCREEN provide a longer period of time over which biodegradation works.

Keywords: AT123D, BIOSCREEN, MODFLOW, MT3D, SESOIL

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1. INTRODUCTION

Groundwater transport modeling can be useful in making informed and defensible remedial decisions. It has been prevalent in the field of environmental hydrogeology because of its wide application in the risk-based decision making process. Often this involves the use of the Domenico equation as a first step of the risk-based process. Selection of an appropriate transport model is of paramount importance in this process, as capabilities and ease of use can vary greatly. This paper compares three commonly used transport models, BIOSCREEN, AT123D, and MODFLOW/MT3D. These models are used to predict groundwater contaminant concentrations, which in turn can determine the amount of contamination that can remain in place while assuring the protection of human health and environment. The three models reviewed in this paper were selected based on their past use and availability.

1.1 Model Description

There are two basic types of computer-based groundwater transport models: analytical and numerical. Analytical models use equations to calculate exact solutions for simple hydrogeological systems, while numerical models provide approximate solutions for complex hydrogeologic conditions.

1.1.1 Analytical Models

AT123D and BIOSCREEN are both analytical groundwater models, and as such they use equations to calculate concentrations at specific locations and times. Results at any point are established independently of results at adjacent points or upon previous time steps. This makes analytical models much easier to use, and eliminates many common problems associated with numerical modeling. For instance, there is no need to design a three-dimensional grid prior to running the model. Furthermore, there is no need to calibrate analytical models. This ease of use has sometimes been misinterpreted as indicating that analytical models are less accurate than numerical models; however, this is not necessarily the case. Instead, the downside related to analytical models is that they are restricted to uniform flow conditions.

1.1.2 Numerical Models

Numerical models, such as MODFLOW/MT3D, provide approximate solutions for complex hydrogeologic conditions. Unlike analytical models, numerical model results depend upon many factors including cell (grid) size and the length of the model stress periods. This makes setting up MODFLOW/MT3D far more complicated than running either BIOSCREEN or AT123D. In general, numerical modeling consists of several steps. First, the area of interest must be divided into a grid of three-dimensional cells. These cells can vary in length, width and thickness. Thus, the grid must be carefully designed, as results are dependent upon cell size. Properties are then assigned to each cell. These properties are assumed to be uniform within a cell, although they can vary from cell to cell. Second, once the grid is established, a method (i.e., Preconditionate

Conjugate Gradient - PCG, Slice Implicit Procedure - SIP, etc.) is selected to solve the finite-difference equations.

It should be noted that results are produced for all model cells, not just the cells of concern, which means that cell size should be small enough to represent a point of compliance but large enough to minimize model run times. In general, accuracy is increased as grid cell sizes decrease. At the same time, the grid must accommodate the contaminant release coordinates. It is not advisable to simply increase the size of the time steps to shorten run times as this may also alter the results. Specifically, if the time step or the grid spacing is too large, the simulation results are poor. Furthermore, the simulation results rely greatly upon the results obtained in adjacent cells and at earlier times. Reducing the values of these parameters may improve the results at the expense of lengthily model run times.

The advantage of numerical models is that they are valid over a wide range of complex hydrological conditions. However, prior to predictive modeling, groundwater flow must be calibrated to site conditions. This means that additional information, including pump tests data, are required for calibration. Calibration is performed by carefully varying input parameters until model results match the observed head values. It should be pointed out that most sites have insufficient data for proper calibration, making it impossible to assure that the models are properly set up. Once MODFLOW is calibrated, the MT3D transport and fate model can be run. Contaminant load in MT3D can be introduced in any of the model cells or at the top of a cell (Figure 1). MT3D results may often indicate a need for further calibration. Finally budgetary constraints and project deadlines may further restrict the use of numerical models.

1.2 BIOSCREEN

In recent years there has been a significant increase of the use of groundwater models based on the Domenico (1987) analytical equation (Table 1). This includes BIOSCREEN (1996), which was developed for the US Air Force by Ground Water Services, Inc. With over 6,000 downloads it may be the most widely used groundwater model in the world. BIOSCREEN is a public domain, two-dimensional screening level groundwater transport and fate model, that is used by many regulatory agencies as a screening model. Contaminant transport is simulated under one-dimensional horizontal groundwater flow. Version 1.4 of the BIOSCREEN model was utilized to perform the modeling in this review.

Table 1. Domenico Equation Based Groundwater Models

RBCA Tool Kit for Chemical Releases v 1.3b	Texas - Update from RBCA for Chemical Releases
RNA Tool Kit for the Florida Petroleum Cleanup Program	FATE5
RBCA Tool Kit for Atlantic Canada v 2.0	BIOSCREEN
Update from version 1.0.1	BUSTR-Screen
Delaware - DERBCAP Module	BIOCHLOR
Delaware - Update from RBCA for Chemical Releases	Illinois EPA TACO
Texas - RBCA Tool Kit for TRRP	

Produced by The Berkeley Electronic Press, 2008

There is only one type of load configuration in BIOSCREEN, in which the contamination is applied as a plane perpendicular to groundwater flow (Figure 1). Processes simulated in this model are advection, dispersion, adsorption, and biological decay (Table 2). Biodegradation can be simulated either a first-order decay or an instantaneous reaction process. The results can be displayed as both area and centerline graphs. However, BIOSCREEN cannot produce a point of compliance report. Aquifer boundaries are set to infinite in BIOSCREEN.

The Domenico equation on which the BIOSCREEN model is based assumes that the source contaminant concentration remains constant through time (i.e. the source mass is infinite) (Figure 2). This means that the source concentration remains constant no matter how long the model is run. The infinite source is an inherent limitation of the Domenico equation that does not depict any real world release scenario. It does however simplify the math thus significantly reducing the computational time. In an attempt to overcome this limitation of the Domenico equation, a declining source concentration term was added to BIOSCREEN. This was accomplished by reducing the source concentration at a rate based on an estimate of the total mass in the source volume (even though actual load is still only a plane). However, the rate at which the source declines is not explicitly determined based on contaminant migration. As stated in the BIOSCREEN User's manual: "this is an experimental relationship, and it should be applied with caution". Most regulatory agencies are aware of the problems associated with the declining source in BIOSCREEN and require that it only be run using the infinite source option.

1.3 AT123D

AT123D (G.T. Yeh 1981) is an acronym for the Analytical Transient 1-, 2-, and 3-Dimensional Simulation of Waste Transport in the Aquifer System. It is a public domain three-dimensional analytical groundwater transport model. Contaminant transport is simulated under one-dimensional horizontal groundwater flow. Transport processes simulated are advection, dispersion, adsorption, diffusion, and biodegradation (Table 2). The aquifer can be simulated as either confined or unconfined.

On the surface AT123D and BIOSCREEN appear to be very similar, yet there are significant differences in the basic model assumptions. For instance BIOSCREEN is written in Excel, which although powerful is not designed to optimize mathematical calculations. On the other hand, AT123D and MODFLOW/MT3D are all written in FORTRAN, which is specifically created for the development of scientific applications. This provides a dramatic improvement in performance, which allows AT123D and MODFLOW/MT3D to simulate a wider array of processes and load configurations.

There are a total of eight load configurations in AT123D, in which the load can be established as a point, line, area or volume (Figure 1). The source concentration in AT123D declines as contamination migrates downgradient (Figure 2). In addition to simulating a single instantaneous release, a separate load for each time-step can be applied in AT123D. This feature allows AT123D to be linked to the SESOIL vadose zone model. The SESOIL - AT123D link is one of the reasons why the SESOIL and AT123D models have been used by a number of state agencies to develop baseline cleanup objectives. Modeling was performed using Version 6.0 of AT123D in the SEVIEW 6.3 Integrated Contaminant Transport and Fate Modeling System

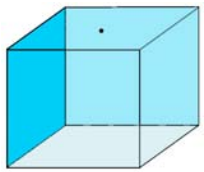
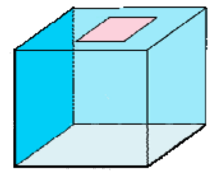
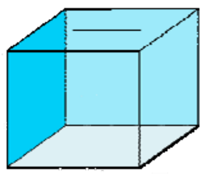
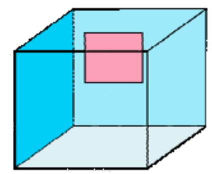
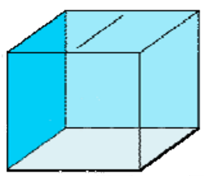
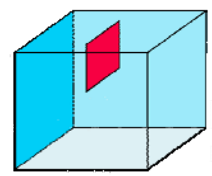
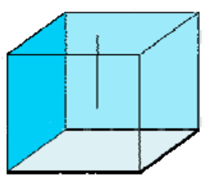
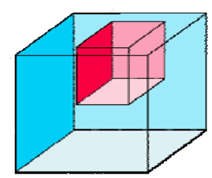
Load		BIOSCREEN	AT123D	MODFLOW MT3D	Load		BIOSCREEN	AT123D	MODFLOW MT3D
Point			✓		Area			✓	✓
Line			✓					✓	
			✓				✓	✓	
			✓		Volume			✓	✓

Figure 1. Model Load Configurations

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Table 2. Model Processes

Process	BIOSCREEN	AT123D	MODFLOW/MT3D
Volume source		✓	✓
Declining source		✓	✓
Advection	✓	✓	✓
Dispersion	✓	✓	✓
Adsorption	✓	✓	✓
Biological Decay	✓	✓	✓
Water Diffusion		✓	✓

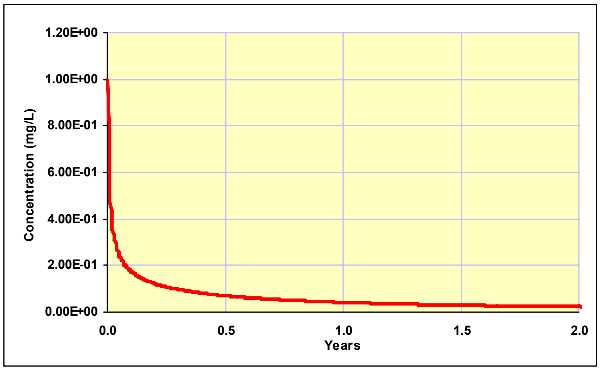
(ESCI, 2005). SEVIEW was used to setup and run the AT123D model. The SEVIEW point of compliance report was used to determine the peak groundwater concentrations.

1.4 MODFLOW and MD3D

MODFLOW (McDonald and Harbaugh 1984) is a public domain three-dimensional numerical groundwater model. Groundwater flow can be simulated for both steady state and transient conditions. It can also simulate flow based on external stresses, such as wells, recharge, evapotranspiration, rivers, and lakes. Hydraulic conductivities, storage coefficients, and groundwater flow parameters may differ spatially (horizontal–specific for each cell, vertical–specific for each layer), thus accounting for anisotropic conditions (heterogeneous aquifers). Specified head and flux boundaries can be used to simulate head inside the boundary domain. The aquifer can be simulated as confined or unconfined. MODFLOW is currently the most widely used numerical model in U.S. for groundwater flow problems.

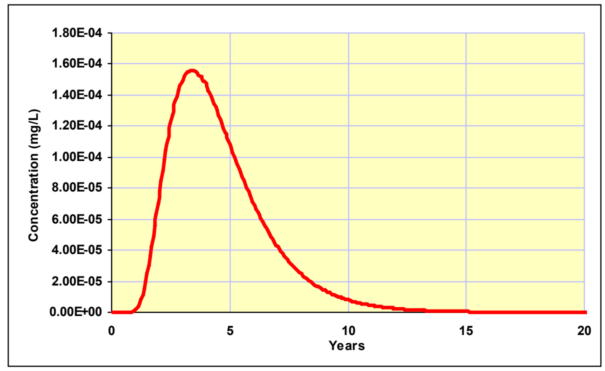
MT3D (C. Zheng 1990) is a public domain three-dimensional transport model. It was developed independently from MODFLOW and was designed to work with any cell-centered numerical groundwater flow model. Transport processes simulated are advection, dispersion, adsorption, diffusion, and biodegradation (Table 2). As with AT123D varying contaminant loads can be applied for each time step. The feature means that MT3D can also be link to the SESOIL model. In addition, MT3D can simulate time-dependent aquifer conditions. Contaminant load can be established as a volume of contaminated groundwater in any of the cells or as a plane at the top of the water table (Figure 1). As with AT123D, MT3D simulates a declining source as an integral part of the transport and fate process. Together MODFLOW and MT3D represent the gold standard in modeling.

Source Concentration



Declining source concentrations as predicted by the AT123D and MT3D models. The source is depleted as the contamination migrates downgradient.

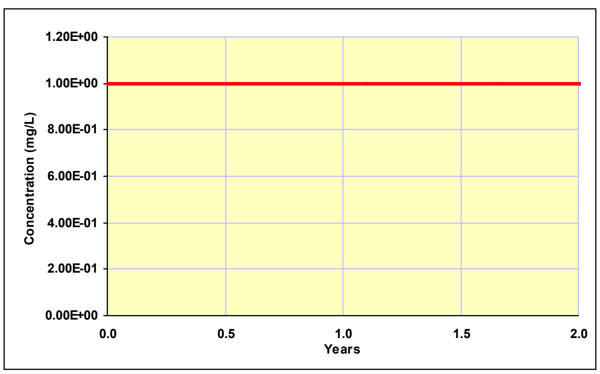
Downgradient Concentration



Resulting downgradient contaminant concentrations reach a peak value then decline due depletion of the source.

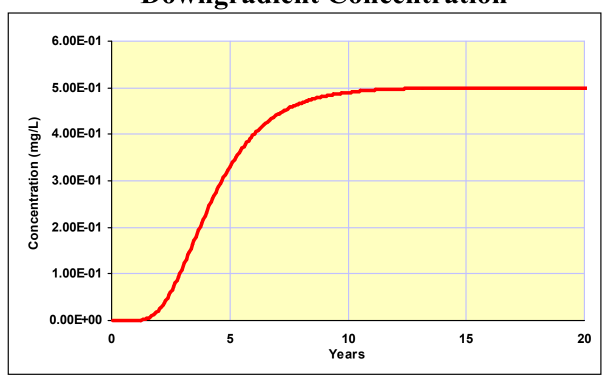
Infinite Load (BIOSCREEN)

Source Concentration



The source concentration remains constant through time. This is because BIOSCREEN does not simulate the depletion of the source.

Downgradient Concentration



Downgradient concentrations reach a peak value but never decline.

Figure 2. Instantaneous Load (AT123D and MODFLOW/MT3D)

1.5 Transport and Fate Processes

Groundwater models use various methods to simulate contaminant transport and fate processes. A summary of transport and fate processes simulated by the models is displayed in

Table 2. There can be substantial differences in the total number of processes simulated and in the methods used to simulate a particular process. All of the models tested simulate advection, dispersion, adsorption, and biological decay processes. The AT123D and MT3D models simulate two additional processes. The first is the declining source concentration as the contamination mass migrates downgradient. The second is the water diffusion process. Water diffusion produces migration of contamination from areas of higher concentration to areas of lower concentration. This process is not dependent upon groundwater flow and as such it even occurs in stagnant groundwater. Diffusion becomes progressively more important as groundwater flow decreases. Inclusion of this process means that AT123D and MODFLOW/MT3D can be used for lower permeability aquifers than BIOSCREEN. Inclusion of the water diffusion coefficient is not an issue, as many regulatory agencies have published values. In addition values can be quickly located in the chemical literature or even calculated based on molecular weight.

1.6 Input Parameters

Model input parameters (Tables 3 and 4) were obtained from default values specified by the Ohio Department of Commerce, Bureau of Underground Storage Tank Regulations (BUSTR, 2003). These input parameters were designed for use in the BUSTRScreen transport and fate model. BUSTRScreen is a variation of BIOSCREEN specifically developed for BUSTR. A tight clay aquifer scenario was added. This produced a wide range of conditions over which model responses could be evaluated. A gradient of 0.001 ft/ft was used for all aquifers. Modeling was performed for benzene and methyl tertiary-butyl ether (MTBE). We decided to use these chemicals as they often control remediation of contaminated sites. Chemical specific parameters for organic carbon partition coefficient (Koc) and water diffusion coefficient were obtained from the SEVIEW 6.3 chemical database. Biodegradation rate values were also obtained from the BUSTR data. Biodegradation of MTBE was not considered, as it is not assumed to readily degrade. Dispersivity values utilized in this evaluation are presented on (Table 5). AT123D and BIOSCREEN input parameters are almost identical with the exception of two additional parameters in AT123D: the distance of the load in the x direction and the water diffusion coefficient (Table 6).

This evaluation consisted of determining predicted groundwater concentrations at a point ten meters (32 feet) downgradient of the source. Hydraulic conductivities simulated ranged from 1.0E+1 cm/sec to 1.0E-6 cm/sec. A total of 54 model scenarios were completed to evaluate results over a wide range of conditions.

1.7 Model Parameters

The source dimensions were set to 6 by 10 by 5 feet in AT123D and MT3D, while the source in BIOSCREEN was set to a plane perpendicular to groundwater flow with a width of 10 feet and a depth of 5 feet (Table 7). Modeling was performed using an initial concentration of 1.0 ppm.

Table 3. Aquifer Parameters

Aquifer Type	Hydraulic Conductivity	Porosity	Bulk Density	Soil Organic Carbon	Gradient
units	cm/sec	dimensionless	kg/L	fraction	ft/ft
Tight Clay	1.0E-6	0.20	1.9	0.001	0.001
Clay	1.0E-5	0.20	1.8	0.001	0.001
Silt	1.0E-3	0.30	1.7	0.001	0.001
Silty Sand	1.0E-1	0.30	1.6	0.001	0.001
Clean Sand	1.0E+0	0.30	1.5	0.001	0.001
Gravel	1.0E+1	0.35	1.4	0.001	0.001

Table 4. Chemical Parameters

Chemical of Concern	Partition Coefficient (K_{oc})	Solute Half-Life	Water Diffusion Coefficient	Maximum Contaminant Level (MCL)
units	L/kg	years	cm^2/sec	mg/L
Benzene	58.9	1.97	9.80E-6	0.005
Methyl-tertiary Butyl Ether	6.0	- -	8.70E-6	0.040

Table 5. Aquifer Dispersivities

units	ft
Longitudinal	3.28
Transverse	0.328
Vertical	0.0328

Table 6. AT123D and BIOSCREEN Input Parameters

1.7.1.1.1 Parameter		BIOSCREEN	AT123D	MODFLOW/MT3D
Hydraulic Conductivity		✓	✓	✓
Gradient		✓	✓	✓
Dispersivities		✓	✓	✓
Porosity		✓	✓	✓
Bulk Density		✓	✓	✓
Organic Carbon Content		✓	✓	✓
Partition Coefficient		✓	✓	✓
Biodegradation	**Half-Life**	✓	✓	✓
	Instantaneous Reaction	✓		
Water Diffusion Coefficient			✓	✓

1.8 Model Setup And Run Times

It took less than 5 minutes to set up each of the BIOSCREEN and AT123D scenarios. It took about two hours to setup the MODFLOW/MT3D models. Modeling was performed using a 2.4 GHz Pentium 4 computer using the Microsoft Windows XP operating system. BIOSCREEN was run in Microsoft Excel 97. Among all three models, BIOSCREEN was the fastest, producing almost instantaneous results for all aquifer types. AT123D came in second taking a maximum of 10 seconds to run. It took MODFLOW/MT3D up to 28 minutes to run the tight clay simulations. Even then, rather than waiting for hours for the run to finish, some of the MODFLOW/MT3D runs were terminated once the peak concentration was observed.

Table 7. Contaminant Load Coordinates

Models	**AT123D & 1.8.1.1 MODFLOW/MT3D**	**BIOSCREEN All**
units	ft	ft
x-axis*	-6.0	0.0
y-axis	10.0 (± 5.0)	
z-axis	-5.0	

1.9 Reports

All three models present results as area reports (Table 8). These reports depict concentrations over the entire area at a specific time. Although the area reports are nicely presented, they provide little relevant data for the evaluation of exposure risk. Both AT123D and BIOSCREEN have centerline reports. This report is particularly useful when calibrating contaminant concentrations to measured values.

Table 8. Model Reporting Capabilities

Parameter	**BIOSCREEN**	**AT123D**	**MODFLOW/MT3D**
Area	✓	✓	✓
Centerline	✓	✓	
Point of compliance		✓	*
* MT3D data is saved as a text file that can be imported in to Excel.			

Both AT123D and MT3D present results at a point of compliance. Called an observation point in MT3D, this report depicts predicted concentrations over time at a specific location, which meets the requirement for the development of risk-based evaluations. BIOSCREEN does not contain a point of compliance report and as such, it had to be run over and over until sufficient output data was produced to create a point of compliance report. It should be noted that this process made BIOSCREEN the slowest model by far.

2. RESULTS

Results show a strong agreement in the peak concentrations and travel times produced by AT123D and MODFLOW/MT3D for all hydraulic conductivities and contaminants tested. However BIOSCREEN results were at least one order of magnitude higher than the other models for hydraulic conductivities between 1.0E+1 cm/sec and 1.0E-3 cm/sec. Predicted concentrations for BIOSCREEN and the other models diverged further as hydraulic conductivities were reduced, reaching a maximum of three orders of magnitude at a hydraulic conductivity of 1.0E-6 cm/sec. It should be noted that BIOSCREEN produced the same peak downgradient concentration for both contaminants and for all hydraulic conductivities. Travel times to peak downgradient concentrations predicted by BIOSCREEN were significantly longer, reaching a maximum of 39,000 years for benzene with a hydraulic conductivity of 1.0E-6 cm/sec. However, based on AT123D and MODFLOW/MT3D predicted travel times were 310 and 572 years respectively.

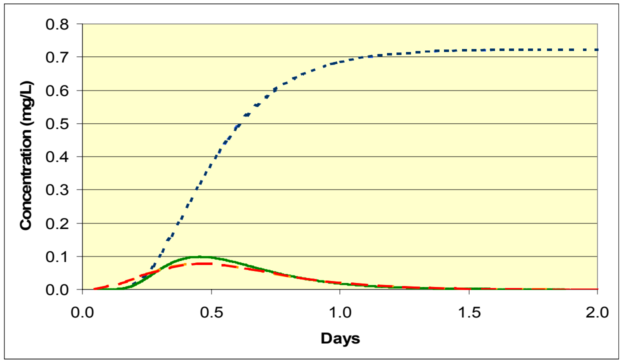
Results were evaluated at a point located 10 meters (32 feet) downgradient from the source. The 10-meter distance was selected because some regulatory agencies have used this distance in the development of default cleanup objectives. Modeling results are presented not only as peak groundwater concentrations, but also as maximum allowable source concentrations. The resulting groundwater concentrations are shown in Tables 9 and 10 (as well as in Figures 3 and 4). Due to the significant difference between the BIOSCREEN results and the other models, concentrations are displayed as both linear and logarithmic plots. Travel times to the peak concentrations are presented in Tables 11 and 12.

In general, the AT123D model results match well with the MODFLOW/MT3D simulations. These models produced almost identical peak concentrations and at nearly the same time. Observed variations may be related to differences in the way in results are established. For example results in AT123D are calculated for a specific point, where as results in MODFLOW/MT3D are generated for an entire cell.

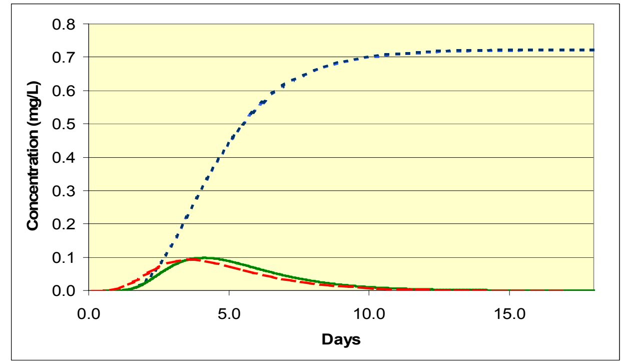
Peak concentrations produced by BIOSCREEN did not vary at all. In fact, BIOSCREEN produced the same peak downgradient concentration for all aquifer types and chemicals tested (Figures 3a to 4b). Additional modeling using benzo-a-pyrene confirmed that BIOSCREEN produces the same peak concentration regardless of the contaminant properties or aquifer type. Travel times varied significantly from the other models taking up to 39,000 years for benzene to reach a point 10 meters downgradient. Where as, AT123D and MODFLOW/MT3D predicted it would only take 310 and 572 years respectively.

According to BIOSCREEN it would take benzene 40 years to reach a point 10 meters downgradient with a hydraulic conductivity of 1.0E-3 cm/sec. However, the other two models indicate it would only take 10 years for benzene to reach this point. BIOSCREEN produced a travel time for benzene of 3,980 years at a hydraulic conductivity of 1.0E-5 cm/sec. While the other models indicated to would only take between 311 and 329 years to reach the peak concentration.

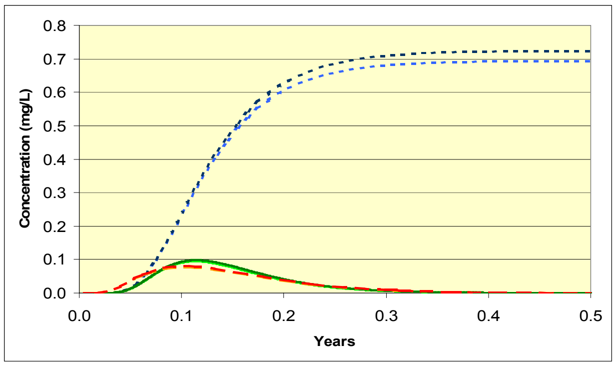
1.0E+1 (cm/sec)



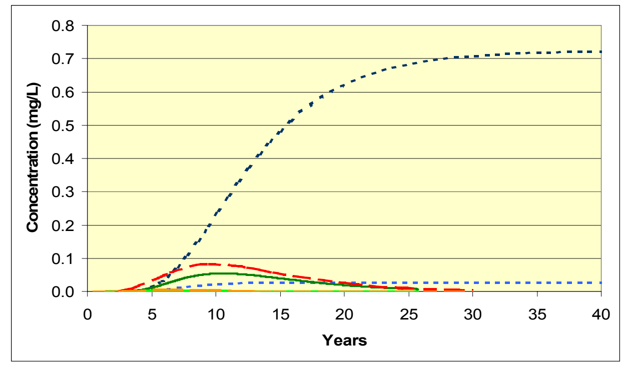
1.0E+0 (cm/sec)



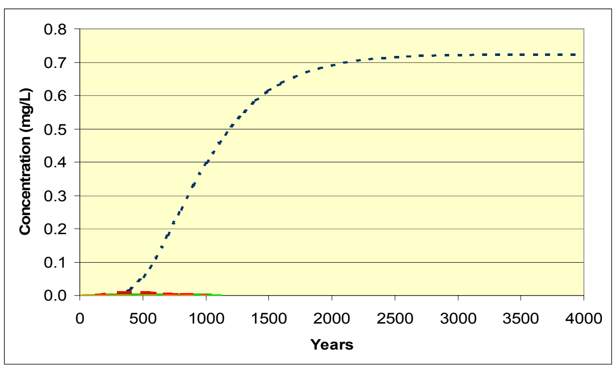
1.0E-1 (cm/sec)



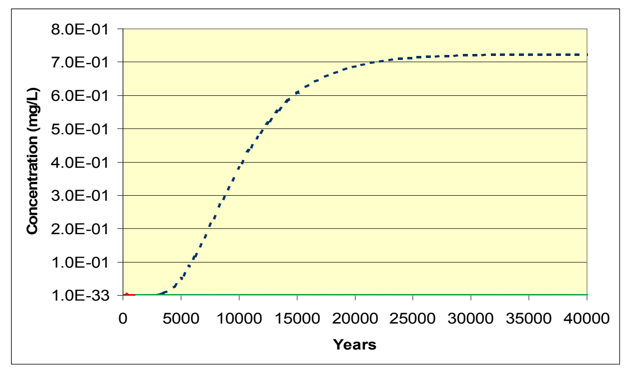
1.0E-3 (cm/sec)



1.0E-5 (cm/sec)



1.0E-6 (cm/sec)



Linear plot of benzene results. BIOSCREEN produced the same peak concentration for all aquifer types. Predicted peak concentrations for the AT123D and MODFLOW/MT3D models were almost identical.

Table 9 Benzene Peak Concentrations

Permeability	BIOSCREEN		AT123D		MODFLOW/MT3D	
	No Bio	w/Bio	No Bio	w/Bio	No Bio	w/Bio
cm/sec	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
1.0E+1	**0.724**	**0.724**	**0.0985**	**0.0985**	**0.0791**	**0.0791**
1.0E+0	**0.724**	**0.721**	**0.0982**	**0.0978**	**0.0934**	**0.0931**
1.0E-1	**0.724**	**0.694**	**0.0982**	**0.0943**	**0.0817**	**0.0788**
1.0E-3	**0.724**	**0.0277**	**0.0543**	**0.00293**	**0.0836**	**0.00581**
1.0E-5	**0.724**	**1.37E-23**	**0.00272**	**3.96E-11**	**0.0108**	**1.05E-12**
1.0E-6	**0.724**	**8.47E-78**	**0.00108**	**8.47E-15**	**0.00242**	**1.48E-15**

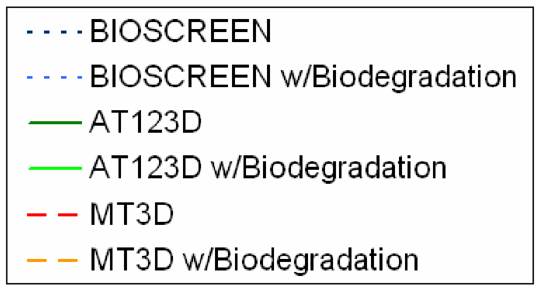
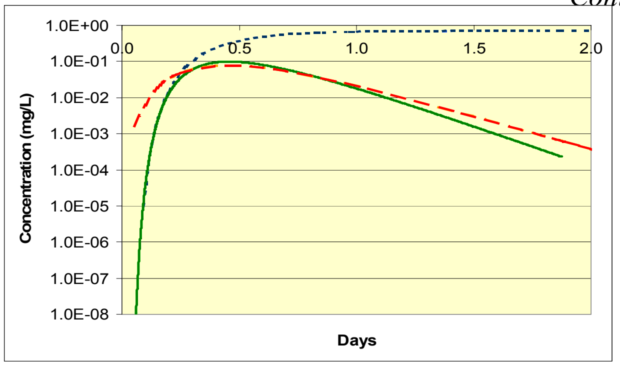
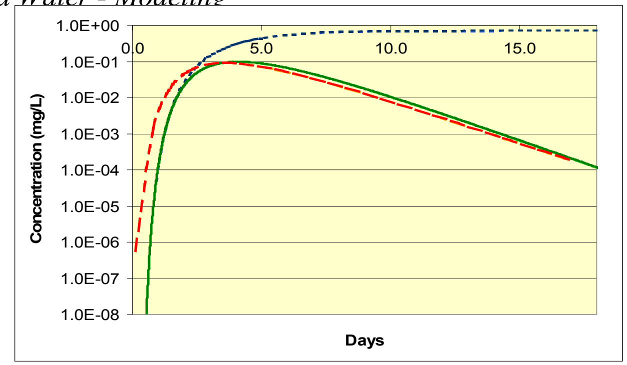


Figure 3a. Linear plots – Benzene Results for Varying Hydraulic Conductivities

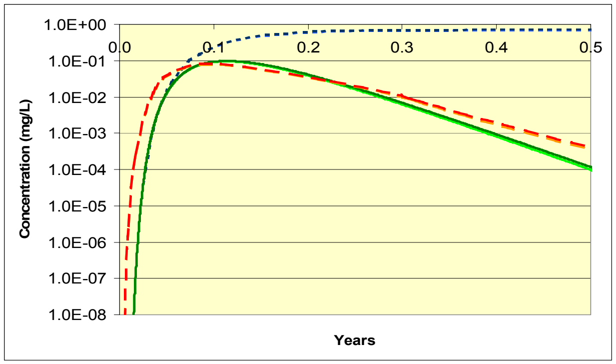
1.0E+1 (cm/sec)



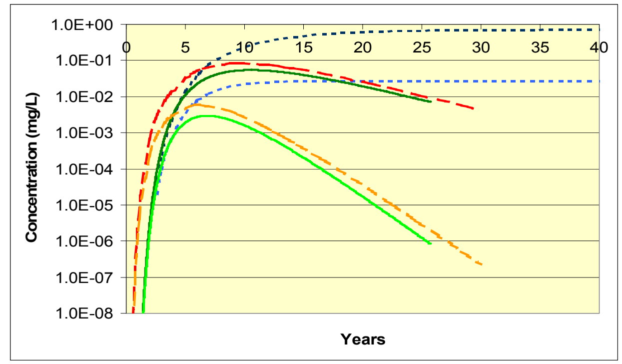
1.0E+0 (cm/sec)



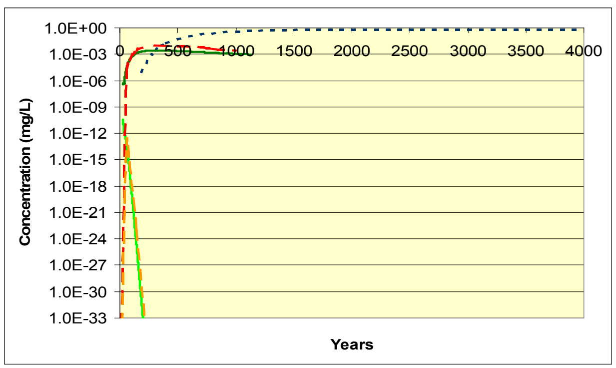
1.0E-1 (cm/sec)



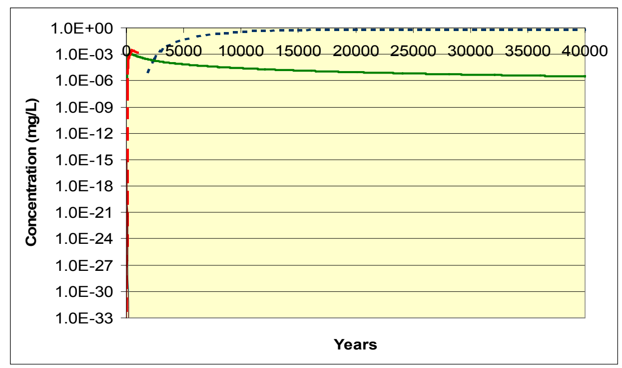
1.0E-3 (cm/sec)



1.0E-5 (cm/sec)



1.0E-6 (cm/sec)



Logarithmic plot of benzene results. BIOSCREEN produced the same peak concentration for all aquifer types. Predicted peak concentrations for the AT123D and MODFLOW/MT3D models were almost identical.

Table 9 Benzene Peak Concentrations

Permeability	BIOSCREEN		AT123D		MODFLOW/MT3D	
	No Bio	w/Bio	No Bio	w/Bio	No Bio	w/Bio
cm/sec	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
1.0E+1	**0.724**	**0.724**	**0.0985**	**0.0985**	**0.0791**	**0.0791**
1.0E+0	**0.724**	**0.721**	**0.0982**	**0.0978**	**0.0934**	**0.0931**
1.0E-1	**0.724**	**0.694**	**0.0982**	**0.0943**	**0.0817**	**0.0788**
1.0E-3	**0.724**	**0.0277**	**0.0543**	**0.00293**	**0.0836**	**0.00581**
1.0E-5	**0.724**	**1.37E-23**	**0.00272**	**3.96E-11**	**0.0108**	**1.05E-12**
1.0E-6	**0.724**	**8.47E-78**	**0.00108**	**8.47E-15**	**0.00242**	**1.48E-15**

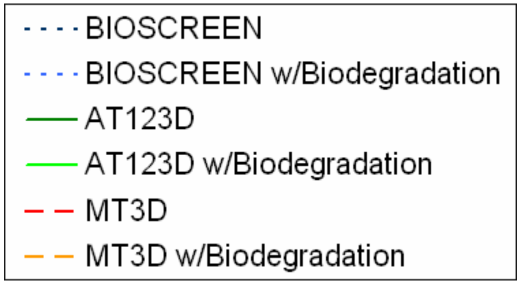
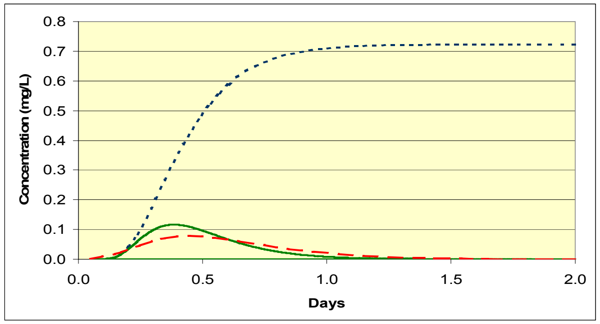
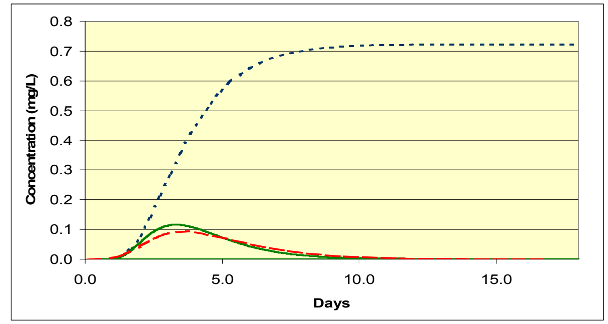


Figure 3b. Logarithmic Plots – Benzene Results for Varying Hydraulic Conductivities

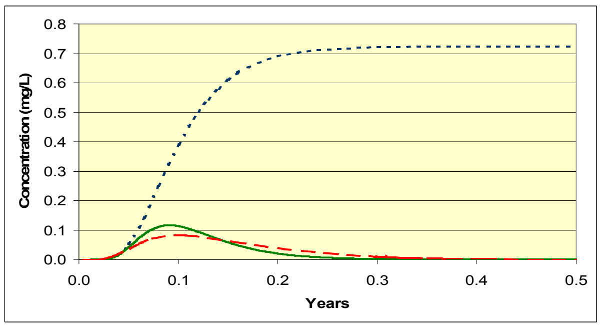
1.0E+1 (cm/sec)



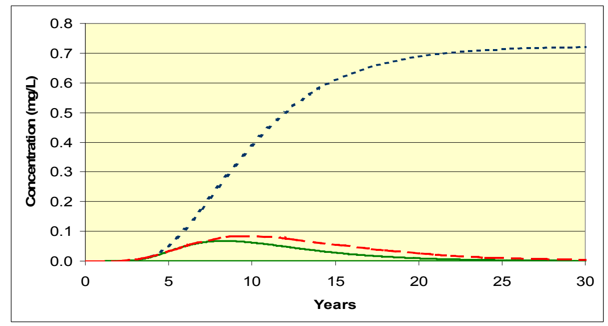
1.0E+0 (cm/sec)



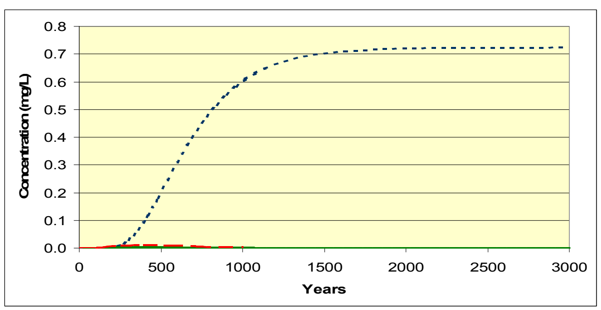
1.0E-1 (cm/sec)



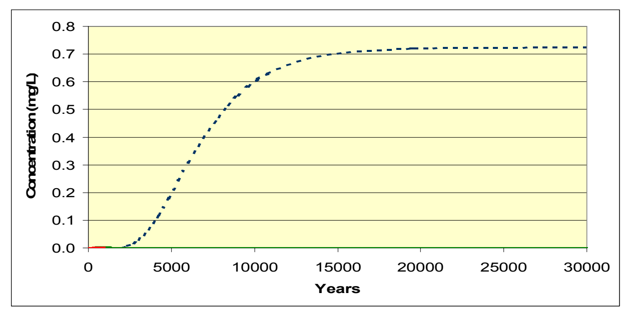
1.0E-3 (cm/sec)



1.0E-5 (cm/sec)



1.0E-6 (cm/sec)



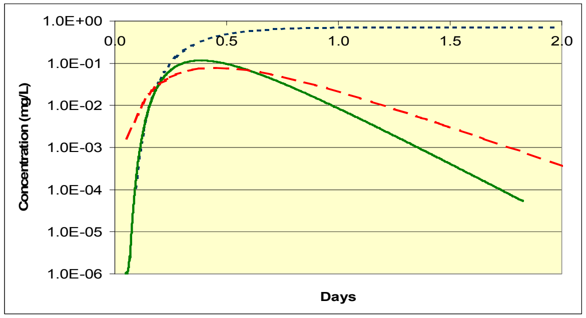
Linear plot of MTBE results. BIOSCREEN produced the same peak concentration for all aquifer types. Predicted peak concentrations for the AT123D and MODFLOW/MT3D models were almost identical.

Table 10 MTBE Peak Concentrations

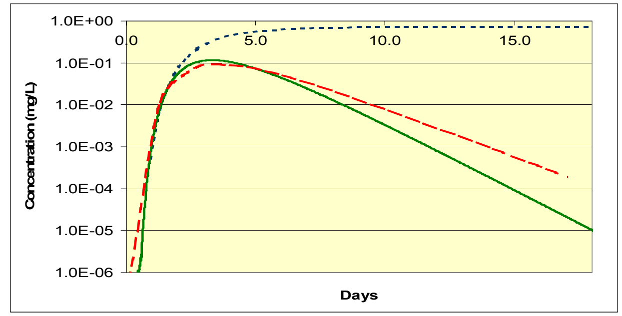
Permeability	BIOSCREEN	AT123D	MODFLOW/MT3D
cm/sec	mg/L	mg/L	mg/L
1.0E+1	0.724	0.116	0.0791
1.0E+0	0.724	0.116	0.0934
1.0E-1	0.724	0.116	0.0817
1.0E-3	0.724	0.0676	0.0847
1.0E-5	0.724	0.00415	0.0120
1.0E-6	0.724	0.00136	0.00251

Figure 4a. Linear plots – MTBE Results for Varying Hydraulic Conductivities

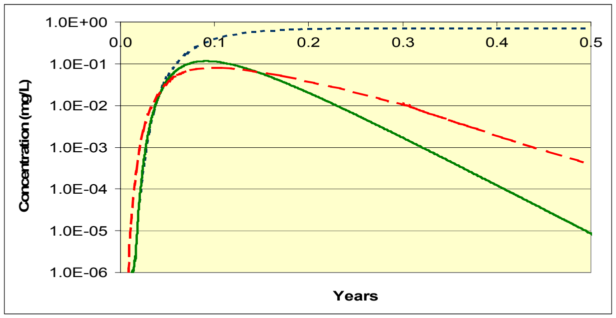
1.0E+1 (cm/sec)



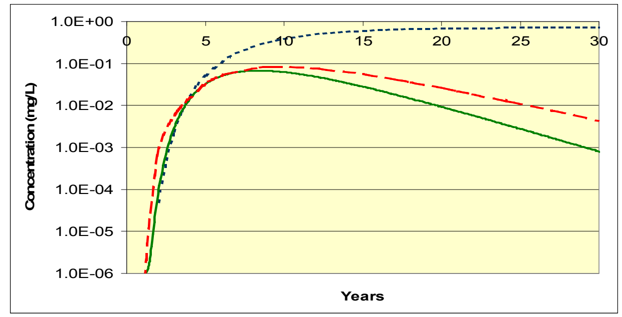
1.0E+0 (cm/sec)



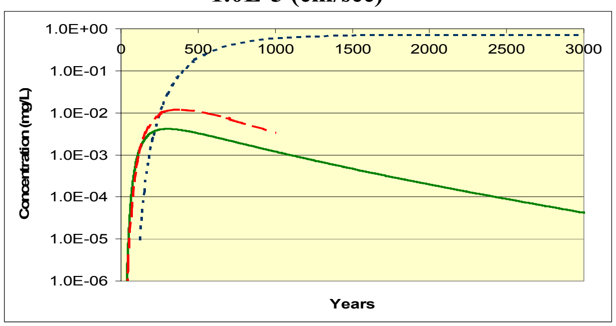
1.0E-1 (cm/sec)



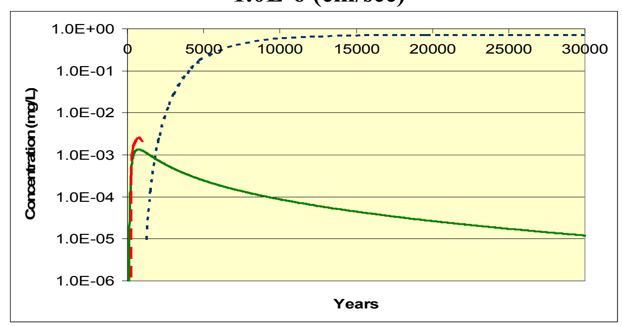
1.0E-3 (cm/sec)



1.0E-5 (cm/sec)



1.0E-6 (cm/sec)



Logarithmic plot of MTBE results. BIOSCREEN produced the same peak concentration for all aquifer types. Predicted peak concentrations for the AT123D and MODFLOW/MT3D models were almost identical.

Table 10 MTBE Peak Concentrations			
Permeability	**BIOSCREEN**	**AT123D**	**MODFLOW/MT3D**
cm/sec	mg/L	mg/L	mg/L
1.0E+1	**0.724**	**0.116**	**0.0791**
1.0E+0	**0.724**	**0.116**	**0.0934**
1.0E-1	**0.724**	**0.116**	**0.0817**
1.0E-3	**0.724**	**0.676**	**0.0847**
1.0E-5	**0.724**	**0.00415**	**0.0120**
1.0E-6	**0.724**	**0.00136**	**0.00251**

Figure 4b. Logarithmic Plots – MTBE Results for Varying Hydraulic Conductivities

Table 11. Time to Peak Benzene Concentrations

Permeability cm/sec	units	BIOSCREEN		AT123D		MODFLOW/MT3D	
		No Bio	w/Bio	No Bio	w/Bio	No Bio	w/Bio
1.0E+1	days	**1.82**	**1.82**	**0.45**	**0.45**	**0.45**	**0.45**
1.0E+0	days	**17.3**	**17.3**	**4.05**	**4.05**	**3.57**	**3.57**
1.0E-1	years	**0.48**	**0.47**	**0.11**	**0.11**	**0.11**	**0.11**
1.0E-3	years	**40**	**23.4**	**10.5**	**6.70**	**9.67**	**6.22**
1.0E-5	years	**3980**	**105**	**311**	**26.3**	**329**	**31.5**
1.0E-6	years	**39000**	**600**	**310**	**50.0**	**572**	**35.9**

Table 12. Time to Peak MTBE Concentrations

Aquifer Type cm/sec	units	BIOSCREEN	AT123D	MODFLOW/MT3D
1.0E+1	days	**1.82**	**0.36**	**0.45**
1.0E+0	days	**15.7**	**3.15**	**3.57**
1.0E-1	years	**0.43**	**0.089**	**0.107**
1.0E-3	years	**43.0**	**8.25**	**9.67**
1.0E-5	years	**2940**	**289**	**359**
1.0E-6	years	**29300**	**680**	**630**

Biodegradation had almost no impact on results for hydrologic conductivities from 1.0E+1 cm/sec to 1.0E-1 cm/sec in any of the models. This is not surprising as it took less than half a year to reach the peak concentration in these aquifers. Such short time frames do not provide enough time for any significant amount of biodegradation. However, at hydraulic conductivities of 1.0E-3 cm/sec and below, biodegradation significantly reduced the resulting peak downgradient concentrations. This is expected as the longer travel times associated with lower permeabilities would give biodegradation a longer period of time over which to work. Given that BIOSCREEN produced the longest travel times, it produced the highest amounts of biodegradation.

2.1 Maximum Allowable Concentrations

The maximum allowable contaminant concentration in the source area is another key point in comparing the results of the three models. Regulations typically require that the predicted groundwater concentrations do not exceed the Maximum Contaminant Level (MCL) at the point of compliance. As demonstrated in (Tables 13 and 14), AT123D and MODFLOW/MT3D allow at least one order of magnitude more benzene and MTBE to remain in place in the source, as did BIOSCREEN for aquifers with hydraulic conductivities of between 1.0E+1 cm/sec and 1.0E-1 cm/sec. As hydraulic conductivities were lowered to 1.0E-6 cm/sec, AT123D and MODFLOW/MT3D allowed up to three orders of magnitude more contamination to remain in the source than BIOSCREEN did.

Table 13. Maximum Allowable Benzene Source Concentrations

Permeability	MCL	BIOSCREEN		AT123D		MODFLOW/MT3D	
		No Bio	w/Bio	No Bio	w/Bio	No Bio	w/Bio
cm/sec	Mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
1.0E+1	**0.005**	**0.00691**	**0.00691**	**0.0508**	**0.0508**	**0.0632**	**0.0632**
1.0E+0	**0.005**	**0.00691**	**0.00693**	**0.0509**	**0.0511**	**0.0535**	**0.0537**
1.0E-1	**0.005**	**0.00691**	**0.00720**	**0.0509**	**0.0530**	**0.0612**	**0.0634**
1.0E-3	**0.005**	**0.00691**	**0.180**	**0.0921**	**1.71**	**0.0598**	**0.860**
1.0E-5	**0.005**	**0.00691**	**3.65E+20**	**1.84**	**1.26E+08**	**0.463**	**4.76E+09**
1.0E-6	**0.005**	**0.00691**	**5.90E+74**	**4.63**	**5.90E+11**	**2.07**	**3.38E+12**

Table 14. Maximum Allowable MTBE Source Concentrations

Permeability	MCL	BIOSCREEN	AT123D	MODFLOW/MT3D
cm/sec	mg/L	mg/L	mg/L	mg/L
1.0E+1	**0.040**	**0.0552**	**0.345**	**0.506**
1.0E+0	**0.040**	**0.0552**	**0.345**	**0.428**
1.0E-1	**0.040**	**0.0552**	**0.345**	**0.490**
1.0E-3	**0.040**	**0.0552**	**0.592**	**0.472**
1.0E-5	**0.040**	**0.0552**	**9.64**	**3.33**
1.0E-6	**0.040**	**0.0552**	**29.4**	**15.9**

Inclusion of biodegradation for benzene had no effect on the maximum allowable source concentration for hydraulic conductivities between 1.0E+1 cm/sec and 1.0E-1 cm/sec in any of the models. This is because the travel times were too short to for biodegradation to produce any effect. However, the influence of biodegradation increased significantly as hydraulic conductivity was lowered. This is due to lengthy travel times associated with the lower hydraulic conductivities. As BIOSCREEN produces the longest travel times it became the least conservative model when biodegradation was included.

2.2 Influence Of Model Capabilities

Discrepancies observed between BIOSCREEN and the other models are not a result of the input parameters. In fact, AT123D and BIOSCREEN use almost identical parameters. Instead the differences are a result of the original model design specifications. BIOSCREEN was designed for ease of use and computational speed. This goal was achieved by limiting contaminant load options, as well as the transport and fate processes. Computation speed was deemed an important design criterion due to limited computer capabilities at that time. Other models, such as AT123D and MODFLOW/MT3D, were initially designed with increased model capabilities, such as additional load options and additional transport and fate processes. Inclusion of these processes in AT123D and MODFLOW/MT3D means that they can be confidently used over a wider range of aquifer types and release scenarios, which in turn, improves confidence in the results. Only recently have computer capabilities improved to the point where run times are no longer an issue for AT123D. Although there has been a significant improvement in performance, model run times still restrict use of the MODFLOW and MT3D models. BIOSCREEN was clearly the fastest model. As far as reporting capabilities both AT123D and MT3D have point of compliance reporting capabilities, making it much faster and easier to evaluate the results.

3. DISCUSSION

With its infinite source concentration, BIOSCREEN produced the most conservative results, if run until the peak concentration is observed. However, even with the infinite source, inclusion of conservative biodegradation rates caused BIOSCREEN to produce the least conservative results. This is because BIOSCREEN does not simulate diffusion, which can become a significant process as gradients and hydraulic conductivities are lowered. Under such conditions BIOSCREEN significantly underestimates contaminant mobility, thus increasing travel times and the amount of biodegradation. Perhaps the most interesting observation is that BIOSCREEN produced the same peak downgradient concentrations for all aquifer types and different chemicals tested. This appears to be intuitively wrong and calls the results in question the basic model assumptions.

There was a strong correlation between the AT123D and MODFLOW/MT3D results. As aquifer and chemical properties changed so did the results. These results are consistent with real world observations.

Ease of use has always been a concern in the process of model selection. Of the three models tested, BIOSCREEN was slightly easier than AT123D to set up and run, while MODFLOW/MT3D is the most challenging. It has often been assumed that more accurate modeling would require additional site characterization to obtain the required input parameters. However, even though AT123D and BIOSCREEN use almost identical input parameters they produce very different results. Our study indicates that improved accuracy is also dependent upon which model is used. That AT123D and MODFLOW produce similar results improves confidence in the reliability of both models.

4. CONCLUSIONS

BIOSCREEN results are not consistent with the other models. When compared to AT123D and MODFLOW/MT3D it significantly under estimates contaminant mobility and over estimates downgradient concentrations. Lengthy travel times produce by BIOSCREEN produce a false sense of security that underestimates exposure risks. Furthermore, given the lengthy travel times, inclusion of even conservative biodegradation rates significantly reduces downgradient concentrations, thus, making BIOSCREEN the least conservative model. Exposure risk is often considered inconsequential at sites where modeling predicts it will take more than 100 years to reach a downgradient point of compliance. Based on our results BIOSCREEN may not be an appropriate model to evaluate such risks.

Risk-based evaluations are established using the peak concentrations and the travel times to reach those peak concentrations. Peak concentrations are used to establish risk-based cleanup levels protective of groundwater quality at the point of compliance. It is typically assumed that risks to groundwater quality decrease as contaminant travel times increase. Therefore, BIOSCREEN, which underestimates contaminant mobility, may not provide an adequate assessment of downgradient risks. Given the lengthy travel times produced by BIOSCREEN, it should always be run until the peak concentration is observed. Even conservative biodegradation rates should be used with caution in BIOSCREEN, as the lengthy travel times produce significantly higher amounts of biodegradation. On the other hand, cleanup objectives based on peak concentrations from BIOSCREEN in which biodegradation is not used are extremely conservative and may result in costly remedial actions, which may not be justified.

Discrepancies are not a result of the model input parameters as AT123D and BIOSCREEN use almost identical parameters. Rather they are a result of inherent limitation associated with BIOSCREEN model and the Domenico equation. Given today's powerful computers, it is difficult to justify the use of BIOSCREEN, especially when AT123D can be safely used over a wider range of aquifer conditions. AT123D produces MODFLOW/MT3D results, yet it takes much less time to use. MODFLOW/MT3D modeling could be performed as an alternative to AT123D modeling. Taking in consideration the costs and complexities associated with numerical modeling may also be advisable to use AT123D to verify the MODFLOW/MT3D results.

5. ACKNOWLEDGEMENTS

We would like to thank James Rumbaugh of Environmental Simulations, Inc. for the use of the Groundwater Vistas software. His assistance was invaluable in the preparation of this paper.

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